4-Ethyltoluene
622-96-8 | DTXSID9029194

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 247

Global applicability domain: Inside

Local applicability domain index: 6.10e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

Image not found
4-Vinylcyclohexene
Measured: 166
Predicted: 158

Image not found
5-Ethylidene-2-norbornene
Measured: 110
Predicted: 134

Image not found
Camphene
Measured: 955
Predicted: 598

Image not found
2,5-Dimethyl-2,4-hexadiene
Measured: 209
Predicted: 175

Image not found
2,4,4-Trimethyl-1-pentene
Measured: 603
Predicted: 347